

REMARKS/ARGUMENTS

The office action issued April 3, 2006 continues the rejection of claim 1 under 35 U.S.C. 102(b). Claims 2-7 remain allowed.

35 U.S.C. 102(b) Rejection

The Examiner has rejected claim 1 under 35 U.S.C. 102(b): "... as being anticipated by International Application Publication Number WO 99/44055 to Nicholls." Specifically, the Examiner states:

With regard to claim 1 Nicholls discloses a computer implemented method to search a heterogeneous compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecules which have the same biological activity as a known query molecule (see abstract) comprising the steps of fragmenting a query molecule and a database molecule according to a defined set of rules (see page 10 line 25), generating shape descriptors for the query molecule and database molecule fragments (see page 22 line 10-19), and using the shape descriptors identifying the database molecule which has a shape similar to the query molecule (see page 25 line 5-26).

In response to the arguments previously presented by Applicants with respect to claim 1, the Examiner states:

Applicant's arguments filed 4-6-2005 have been fully considered but they are not persuasive.

In response to applicant's argument regarding claim 1 that the references fail to show

certain features of applicant's invention, it is noted that the features upon which applicant relies (i.e., matching a "whole" query molecule) are not recited in the rejected claim(s). Although the claims are interpreted in light of the specification, limitations from the specification are not read into the claims. See *In re Van Geuns*, 988 F.2d 1181,26 USPQ2d 1057 (Fed. Cir. 1993). If applicant wishes to limit the scope of the claim to include only whole database molecule and whole query molecule, this feature should be explicitly recited in the claim.

Applicants' Response:

Applicants respectfully continue to believe that the Examiner's analysis is incorrect and present the following further argument. First, Applicants note that they have interpreted the following sentence of the Examiner's action to include the additional word "whole:"

Although applicant argues that an accepted meaning of the word query molecule is "whole" query molecule, the term "whole" query molecule does not appear in the claim.

Applicants have been puzzled why the Examiner has suggested that it is necessary for Applicants to insert the word "whole" in their claim. Applicants note, however, that in their April 6, 2005 office action response they stated that:

Nicholls teaches that he can (shape) match subparts of one molecule with subparts of another molecule or that he can (shape) match a subpart of one molecule with another whole molecule. Nicholls is not concerned with finding a (shape) match of a whole query molecule to a whole database molecule using fragments. Yet, this is precisely what applicants teach. Applicants' method identifies the molecules in the heterogenous

compound database which have the same shape as the query molecule by examining the shape comparisons between fragments of the query molecule and fragments of the database molecule. The method identifies the most similarly shaped database molecule as that molecule having the smallest field value differences in its fragments (compared to the fragments of the query molecule). In other words, applicants use fragments to compare whole molecules to whole molecules. This is the requirement of applicants' method stated in step 1.(c). For this reason, Nicholls can not anticipate applicants' invention. Accordingly, applicants respectfully request the Examiner to remove the 35 U.S.C. 102(b) rejection.

Applicants have reviewed claim 1 in light of the Examiner's remarks and in light of the previously presented argument and have noted that it is potentially possible to parse step 1(b) in two different ways. A first way would read the step to generate shape descriptors for the (whole) query molecule and additional shape descriptors for the database molecule fragments as in:

- b) generating shape descriptors for the query molecule and (for) database molecule fragments

The second way would read the step to generate shape descriptors for both the query molecule fragments and the database molecule fragments as in:

- b) generating shape descriptors for the query molecule (fragments) and database molecule fragments

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It is this second way that was intended by Applicants. Reading step b) in this manner makes clear that shape descriptors of the query molecule fragments and shape descriptors of the data base molecule fragments are used in step c) to identify the database molecule which has a shape similar to the query molecule. Any ambiguity presented by the first parsing of step b), which could be taken to mean that a shape descriptor of a whole query molecule is utilized, is, therefore, removed.

Claim step 1(b) has been amended for clarity to reference that fragments of both the query molecule and the database molecules are generated. Claim step 1(b) has also been amended to make clearer that fragments of database molecules (plural) are generated. Applicants submit that with the amendment, the Examiner's suggestion to recite a "whole query molecule" is no longer necessary, and that claim 1 is now in condition for allowance.

An RCE has been submitted to permit consideration of the claim amendment and argument since this is a response to a final office action. Applicants respectfully request the Examiner to pass the application to issue.

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Respectfully submitted,



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